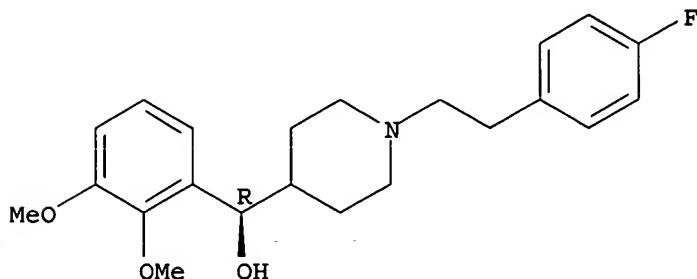


=> s mdl 100907/cn  
L14 1 MDL 100907/CN

=> d

L14 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 139290-65-6 REGISTRY  
ED Entered STN: 28 Feb 1992  
CN 4-Piperidinemethanol,  $\alpha$ -(2,3-dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 4-Piperidinemethanol,  $\alpha$ -(2,3-dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-, (R)-  
OTHER NAMES:  
CN (+)- $\alpha$ -(2,3-Dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-4-piperidinemethanol  
CN (+)-MDL 100907  
CN M 100907  
CN MDL 100907  
CN R-MDL 100907  
FS STEREOSEARCH  
MF C22 H28 F N O3  
CI COM  
SR CA  
LC STN Files: ADISINSIGHT, ADISNEWS, ANABSTR, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, PHAR, PROUSDDR, RTECS\*, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

187 REFERENCES IN FILE CA (1907 TO DATE)  
3 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
187 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
7.10	145.10

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
0.00	-4.50

CA SUBSCRIBER PRICE

FILE 'CAPLUS' ENTERED AT 15:39:18 ON 02 AUG 2006

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FILE LAST UPDATED: 1 Aug 2006 (20060801/ED)

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=> s l14

L15 187 L14

=> s l15(1)metabol?

888348 METABOL?

L16 2 L15 (L)METABOL?

=> d bib abs hitstr 1-2

L16 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1998:313969 CAPLUS

DN 129:49176

TI Investigation of the CNS penetration of a potent 5-HT<sub>2a</sub> receptor antagonist (MDL 100,907) and an active metabolite (MDL 105,725) using in vivo microdialysis sampling in the rat

AU Scott, Dennis O.; Heath, Timothy G.

CS Hoechst Marion Roussel, Inc, Kansas City, MO, 64134-0627, USA

SO Journal of Pharmaceutical and Biomedical Analysis (1998), 17(1), 17-25

CODEN: JPBADA; ISSN: 0731-7085

PB Elsevier Science B.V.

DT Journal

LA English

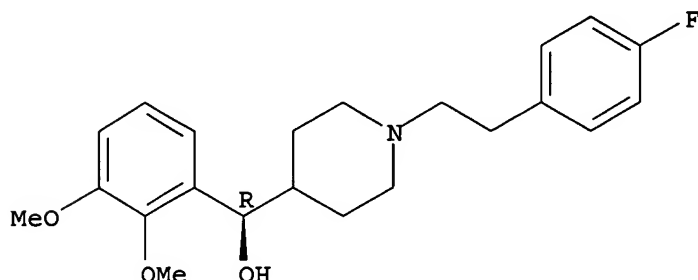
AB MDL 100,907 is a selective 5-HT<sub>2a</sub> receptor antagonist which is currently being developed for the treatment of schizophrenia. Pharmacokinetic studies of MDL 100,907 in rats and dogs show that the drug is well absorbed but undergoes extensive first-pass metabolism to an active metabolite (MDL 105,725). The purpose of this study was to determine concns. of MDL 100,907 and MDL 105,725 in the brain extracellular fluid (ECF) after administration of MDL 100,907. In vivo microdialysis sampling was used to determine the brain penetration of both parent (MDL 100,907) and metabolite (MDL 105,725). Animals (n = 3/dose) were given 5 i.v. and 50 mg kg<sup>-1</sup> oral doses of MDL 100,907. Brain medial prefrontal cortex (mPFC) ECF concns. were determined using microdialysis and plasma levels were determined by collecting

blood samples through an indwelling cannula implanted in the jugular vein. Dialyzate samples were analyzed using an LC/MS/MS assay. The data presented in this report show that the blood brain barrier (BBB) permeability of MDL 100,907 is more than four times (4 +) that of MDL 105,725 and that MDL 100,907 does not undergo significant metabolism to MDL 105,725 in the brain. It appears, from the data presented, that MDL 100,907 is the predominant active species present in the brain at high

doses.

IT 139290-65-6, MDL 100907  
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)  
(CNS penetration of 5-HT<sub>2a</sub> receptor antagonist MDL 100,907 and active metabolite MDL 105,725)  
RN 139290-65-6 CAPLUS  
CN 4-Piperidinemethanol,  $\alpha$ -(2,3-dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

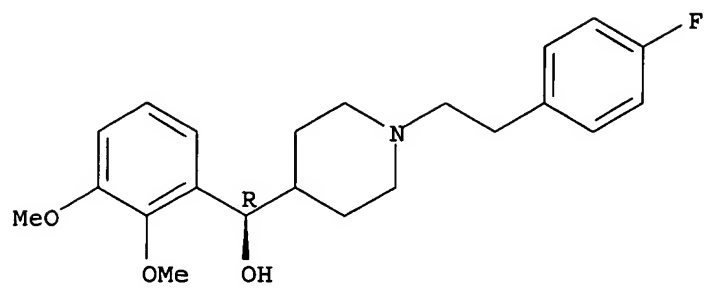
Absolute stereochemistry. Rotation (+).



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

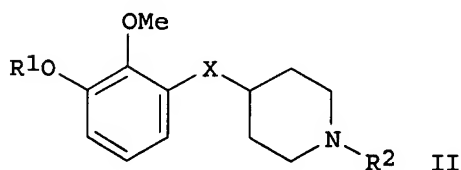
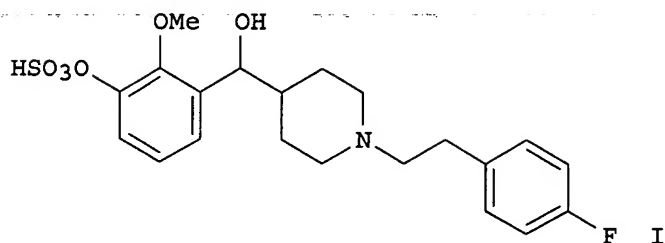
L16 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN  
AN 1997:239223 CAPLUS  
DN 126:287509  
TI Quantification of a potent 5-HT<sub>2a</sub> antagonist and an active metabolite in rat plasma and brain microdialyzate by liquid chromatography-tandem mass spectrometry  
AU Heath, Timothy G.; Scott, Dennis O.  
CS Hoechst Marion Roussel, Kansas City, MO, 64134-0627, USA  
SO Journal of the American Society for Mass Spectrometry (1997), 8(4), 371-379  
CODEN: JAMSEF; ISSN: 1044-0305  
PB Elsevier  
DT Journal  
LA English  
AB A method based on liquid chromatog.-tandem mass spectrometry and microbore column separation was developed for the quantification of a potent 5-HT<sub>2a</sub> receptor antagonist, MDL 100,907 [(R)-(+)- $\alpha$ -(2,3-dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-4-piperidinemethanol] (I) and its demethyl metabolite (II) in rat brain extracellular fluid (ECF) following microdialysis sampling. The method was also applied to determining plasma concns. of these compds. The lower limit of quantification (LLQ) for each compound in the microdialysis perfusate is 500 pg/mL, which translates to <7 fmol (injected). The recovery of I and II from the microdialysis probe in brain ECF was 18.5 and 22.7%, resp. The LLQ for each compound in plasma was 1 ng/mL. The inherent selectivity offered by tandem mass spectrometry eliminated chemical noise, thereby improving the detectability of these compds. These methods were used to confirm that I and II penetrated the blood-brain barrier following administration of I to rats and enabled comparison of plasma and brain ECF concns.  
IT 139290-65-6, MDL 100907  
RL: ANT (Analyte); ANST (Analytical study)  
(determination of serotonergic S<sub>2a</sub> antagonist MDL 100,907 and its demethyl metabolite in brain extracellular fluid and plasma by liquid chromatog.-mass spectrometry)  
RN 139290-65-6 CAPLUS  
CN 4-Piperidinemethanol,  $\alpha$ -(2,3-dimethoxyphenyl)-1-[2-(4-fluorophenyl)ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AN 2001:63973 CAPLUS  
 DN 134:115860  
 TI Preparation of sulfuric acid mono-[3-({1-[2-(4-fluoro-phenyl)-ethyl]-piperidin-4-yl}-hydroxy-methyl)-2-methoxy-phenyl]ester and analogs for use as serotonin 5HT2A receptor antagonists  
 IN Bernotas, Ronald; Brown, Paul; Emmons, Gary; King, Chi-Hsin  
 PA Aventis Pharmaceuticals Inc., USA  
 SO PCT Int. Appl., 54 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001005764	A2	20010125	WO 2000-US19065	20000713
	WO 2001005764	A3	20011004		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	CA 2374635	AA	20010125	CA 2000-2374635	20000713
	BR 2000012477	A	20020402	BR 2000-12477	20000713
	EP 1202967	A2	20020508	EP 2000-947304	20000713
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			
	JP 2003505374	T2	20030212	JP 2001-511425	20000713
	AU 769484	B2	20040129	AU 2000-60939	20000713
	NZ 516286	A	20040326	NZ 2000-516286	20000713
	ZA 2002000101	A	20030404	ZA 2002-101	20020104
	NO 2002000213	A	20020222	NO 2002-213	20020115
PRAI	US 1999-354704	A2	19990716		
	WO 2000-US19065	W	20000713		
OS	MARPAT 134:115860				
GI					



AB Preparation of the title compound I and its analogs II (R1 = H, trialkylsilane,

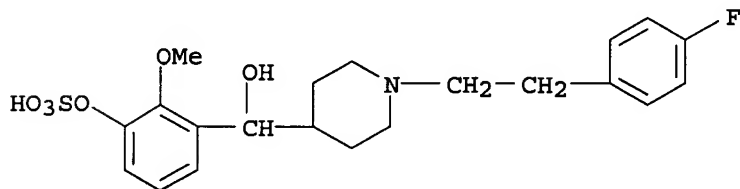
alkylcarboxy; R2 = (un)substituted arylalkyl, COOR3, H; R3 = alkyl, aryl or arylalkyl; X = CO or CHOR4; R4 = H or alkylcarboxy) is disclosed. Thus, compound I was prepared by combined sulfonation/deacetylation of acetic acid {1-[2-(4-fluorophenyl)-ethyl]-piperidin-4-yl}-(3-hydroxy-2-methoxyphenyl)methyl ester. I is an active metabolite of II (R1 = Me; X = CHOH; R2 = 4-FC6H4CH2CH2) and a method for its preparation and isolation via metabolism is claimed. The title compds. are claimed as serotonin 5HT2A receptor antagonists and as such are useful for the treatment of a number of disease states, e.g. schizophrenia, anxiety, variant angina, anorexia nervosa, cardiac arrhythmias, etc.

IT 321547-54-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); USES (Uses)  
(preparation and metabolic formation of the active metabolite sulfuric acid mono[({[fluorophenylethyl]piperidinyl}hydroxymethyl)methoxyphenyl] ester)

RN 321547-54-0 CAPLUS

CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]- $\alpha$ -[2-methoxy-3-(sulfooxy)phenyl]- (9CI) (CA INDEX NAME)

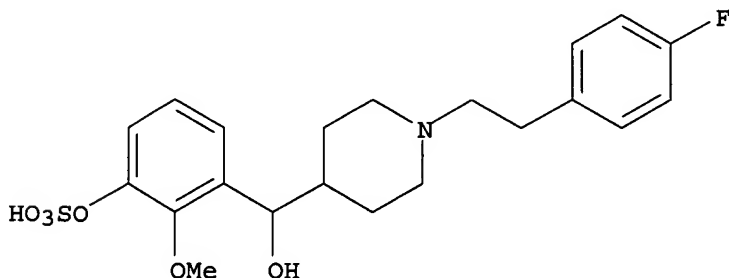


IT 321547-50-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(stereoselective preparation and metabolic formation of the active metabolite sulfuric acid mono[({[fluorophenylethyl]piperidinyl}hydroxymethyl)methoxyphenyl] ester)

RN 321547-50-6 CAPLUS

CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]- $\alpha$ -[2-methoxy-3-(sulfooxy)phenyl]-, (+)- (9CI) (CA INDEX NAME)



Rotation (+).

IT 321547-58-4P

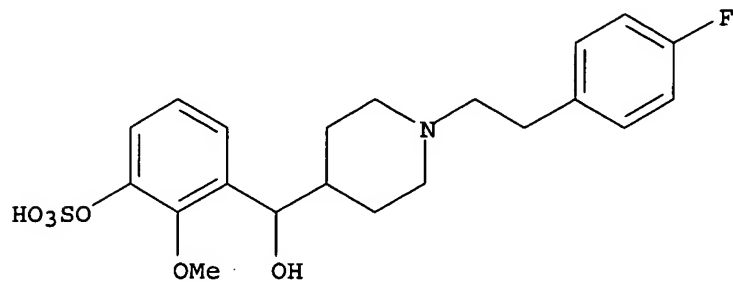
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); MFM (Metabolic formation); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); USES (Uses)

(stereoselective preparation and metabolic formation of the active metabolite sulfuric acid mono[({[4-fluorophenylethyl]piperidinyl}hydroxyethyl)methoxyphenyl] ester)

RN 321547-58-4 CAPLUS

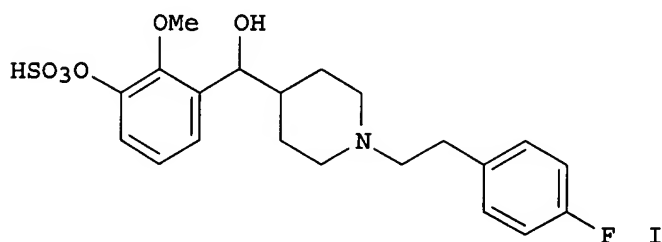
CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]- $\alpha$ -[2-methoxy-3-(sulfooxy)phenyl]-, (-)- (9CI) (CA INDEX NAME)

Rotation (-).



AN 2002:790226 CAPLUS  
 DN 137:310813  
 TI Preparation of sulfuric acid mono-[3[[1-[2-(4-fluorophenyl)ethyl]-piperidin-4-yl]hydroxymethyl]-2-methoxyphenyl]ester and enantiomers as 5HT2A antagonists.  
 IN Bernotas, Ronald Charles; Brown, Paul Wayne; Emmons, Gary Thomas; King, Chi-hsin Richard  
 PA Aventis Pharmaceuticals Inc., USA  
 SO U.S., 19 pp.  
 CODEN: USXXAM  
 DT Patent  
 LA English  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6465490	B1	20021015	US 2000-615246	20000713 <--
	US 2003087932	A1	20030508	US 2002-200821	20020722
	US 6716986	B2	20040406		
	US 2004152900	A1	20040805	US 2004-760515	20040120
PRAI	US 1999-198215P	P	19990716		
	US 2000-615246	A3	20000713		
	US 2002-200821	A3	20020722		
OS	CASREACT 137:310813				
GI					



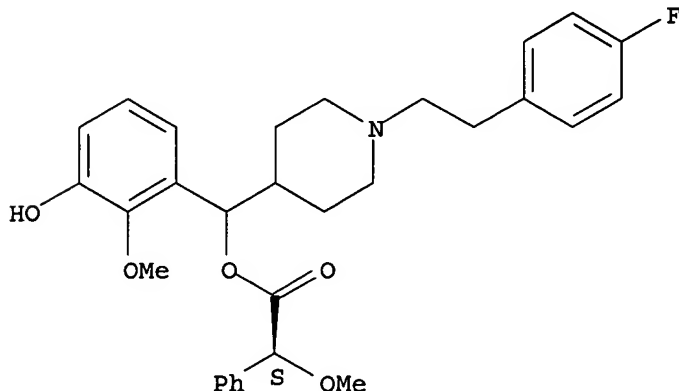
AB Title compds. I were prepared Thus, acetic acid [1-[2-(4-fluorophenyl)ethyl]piperidin-4-yl] (3-hydroxy-2-methoxyphenyl)methyl ester (preparation given) was heated at 45° with SO3.pyridine in MeCN for 18 h; H2O, MeOH, and K2CO3 were added followed by 12 h reflux to give sulfuric acid mono-(+)-[3[[1-[2-(4-fluorophenyl)ethyl]piperidin-4-yl]hydroxymethyl]-2-methoxyphenyl] ester. Title compds. were shown to penetrate the blood-brain barrier.

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT



L8 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
 RN 321547-55-1 REGISTRY  
 ED Entered STN: 13 Feb 2001  
 CN Benzeneacetic acid,  $\alpha$ -methoxy-, [1-[2-(4-fluorophenyl)ethyl]-4-piperidinyl] (3-hydroxy-2-methoxyphenyl)methyl ester, ( $\alpha$ S) - (9CI)  
 (CA INDEX NAME)  
 FS STEREOSEARCH  
 MF C30 H34 F N O5  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

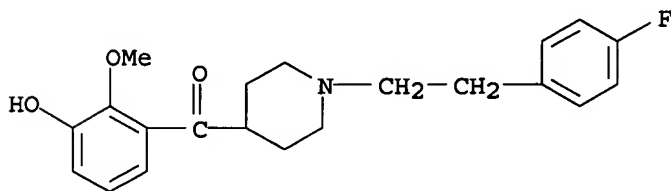
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
 RN 321547-53-9 REGISTRY  
 ED Entered STN: 13 Feb 2001  
 CN Methanone, [1-[2-(4-fluorophenyl)ethyl]-4-piperidinyl] (3-hydroxy-2-methoxyphenyl) - (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C21 H24 F N O3  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

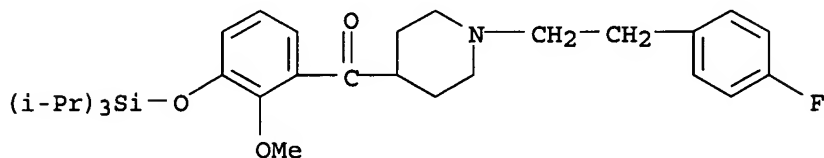


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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L8 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
 RN 321547-52-8 REGISTRY

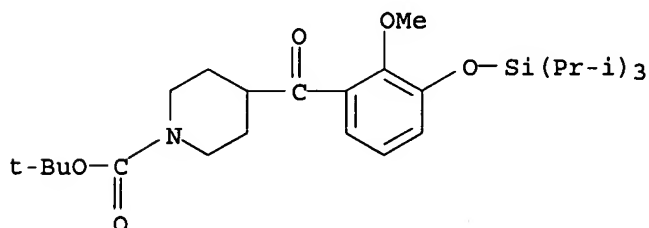
ED Entered STN: 13 Feb 2001  
 CN Methanone, [1-[2-(4-fluorophenyl)ethyl]-4-piperidiny] [2-methoxy-3-  
 [[tris(1-methylethyl)silyl]oxy]phenyl]- (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C30 H44 F N O3 Si  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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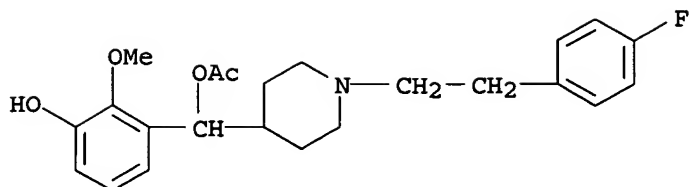
L8 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
 RN 321547-51-7 REGISTRY  
 ED Entered STN: 13 Feb 2001  
 CN 1-Piperidinecarboxylic acid, 4-[2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]benzoyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C27 H45 N O5 Si  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
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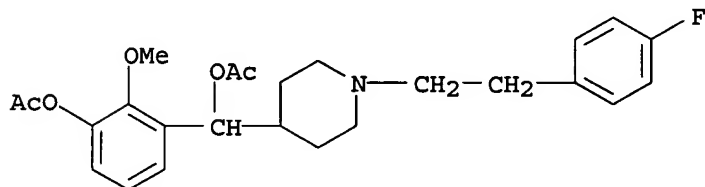
L8 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
 RN 321547-49-3 REGISTRY  
 ED Entered STN: 13 Feb 2001  
 CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]-α-(3-hydroxy-2-methoxyphenyl)-, monoacetate (ester) (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C23 H28 F N O4  
 SR CA  
 LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 321547-48-2 REGISTRY  
ED Entered STN: 13 Feb 2001  
CN 4-Piperidinemethanol,  $\alpha$ -[3-(acetyloxy)-2-methoxyphenyl]-1-[2-(4-fluorophenyl)ethyl]-, acetate (ester) (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C25 H30 F N O5  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

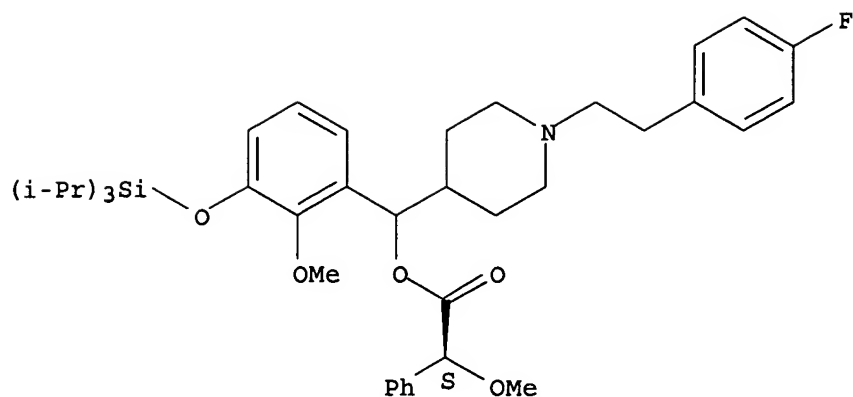


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 321547-47-1 REGISTRY  
ED Entered STN: 13 Feb 2001  
CN Benzeneacetic acid,  $\alpha$ -methoxy-, [1-[2-(4-fluorophenyl)ethyl]-4-piperidinyl][2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]phenyl]methyl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C39 H54 F N O5 Si  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

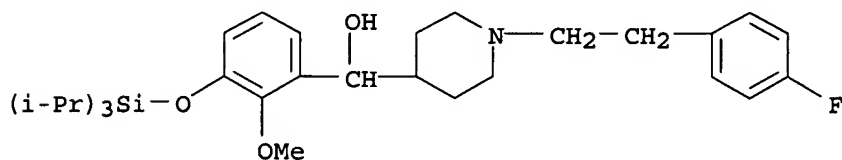
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

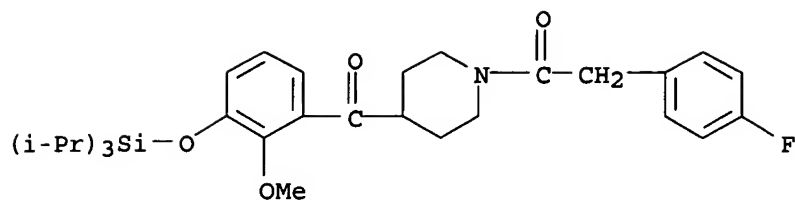
L8 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 321547-46-0 REGISTRY  
ED Entered STN: 13 Feb 2001  
CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]- $\alpha$ -[2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]phenyl]- (9CI) (CA INDEX NAME)  
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MF C30 H46 F N O3 Si  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 321547-45-9 REGISTRY  
ED Entered STN: 13 Feb 2001  
CN Piperidine, 1-[(4-fluorophenyl)acetyl]-4-[2-methoxy-3-[[tris(1-methylethyl)silyl]oxy]benzoyl]- (9CI) (CA INDEX NAME)  
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MF C30 H42 F N O4 Si  
SR CA  
LC STN Files: CA, CAPLUS, CASREACT, USPAT2, USPATFULL

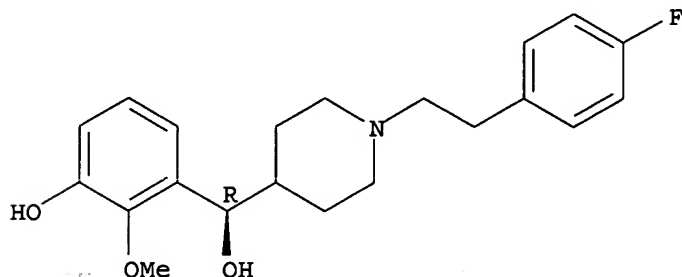


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L8 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2006 ACS on STN  
RN 189192-18-5 REGISTRY  
ED Entered STN: 22 May 1997  
CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]- $\alpha$ -(3-hydroxy-2-methoxyphenyl)-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN 4-Piperidinemethanol, 1-[2-(4-fluorophenyl)ethyl]- $\alpha$ -(3-hydroxy-2-methoxyphenyl)-, (R)-  
OTHER NAMES:  
CN (+)-MDL 105725  
CN MDL 105725  
FS STEREOSEARCH  
MF C21 H26 F N O3  
SR CA  
LC STN Files: BIOSIS, CA, CAPLUS, CASREACT, USPAT2, USPATFULL

Absolute stereochemistry. Rotation (+).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

9 REFERENCES IN FILE CA (1907 TO DATE)  
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

(FILE 'HOME' ENTERED AT 15:31:08 ON 02 AUG 2006)

FILE 'CAPLUS' ENTERED AT 15:31:18 ON 02 AUG 2006

L1 1 S US6465490/PN

L2 ANALYZE L1 1 RN : 20 TERMS

FILE 'REGISTRY' ENTERED AT 15:31:36 ON 02 AUG 2006

L3 20 S L2

L4 14 S L3 AND PIPERIDIN?

L5 3 S L4 AND SULFO?

L6 11 S L4 NOT L5

L7 1 S 139290-70-3

L8 10 S L6 NOT L7

FILE 'CAPLUS' ENTERED AT 15:33:18 ON 02 AUG 2006

L9 9 S L8

L10 3 S L9 AND METABO?

FILE 'REGISTRY' ENTERED AT 15:35:05 ON 02 AUG 2006